

Fluctuation-dissipation relations and critical quenches in the transverse field Ising chain

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(Dated: August 1, 2011)

Dynamic correlation and response functions of classical and quantum systems in thermal equilibrium are connected by fluctuation-dissipation theorems, which allow an alternative definition of their (unique) temperature. Motivated by this fundamental property, we revisit the issue of thermalization of closed many-body quantum systems long after a sudden quench, focussing on the non-equilibrium dynamics of the Ising chain in a critical transverse field. We show the emergence of distinct observable-dependent effective temperatures, which rule out Gibbs thermalization in a strict sense but might still have a thermodynamic meaning.

Introduction. The development of experimental techniques which prevent dissipation in quantum many-body systems has triggered increasing interest in the non-equilibrium dynamics of such closed systems. The unitary non-equilibrium dynamics of a system initially prepared in a state which is not an eigenstate of its Hamiltonian is called a *quantum quench*. Basic questions as to whether a stationary state is reached and how this can be characterized naturally arise. These questions have been addressed in a number of simple models, including the one-dimensional systems reviewed in Refs. [1, 2]. Early studies led to the following picture: Non-integrable systems should eventually reach a thermal stationary state characterized by a Gibbs distribution with a single temperature. Integrable systems, instead, are not expected to thermalize but their asymptotic stationary state should nonetheless be described by a so-called generalized Gibbs ensemble (GGE) with one effective temperature for each conserved quantity [3–6]. Interestingly enough, depending on the specific quantity and the system’s parameters a Gibbs ensemble turns out to capture anyhow some relevant features of the non-equilibrium dynamics of integrable systems [7]. In particular, observables that are non-local in the quasi-particles display numerically the same relaxation scales as in equilibrium with a suitable effective temperature, at least for small quenches [6, 7]. Local quantities instead do not, with possible exceptions for quenches at criticality.

Our purpose is to revisit the debated issue of thermalization in closed quantum systems with tools developed for the study of *classical and quantum dissipative glassy systems*. The analysis of thermalization in closed quantum systems focused so far on the property that expectation values of quantities — such as (i) the conserved energy and two-point correlation functions depending on either (ii) one or (iii) two times — should behave, at long times, as the corresponding averages calculated on suitable statistical ensembles. However, an equally im-

portant property of thermal equilibrium states of both classical and quantum systems is the validity of model-independent fluctuation-dissipation theorems (FDTs) [8], which relate *linear response and correlation functions* independently of their functional form. Focusing on two-time quantities, we investigate thermalization issues from this perspective.

Before getting into the technical details, let us explain why fluctuation-dissipation relations (FDRs) should be more relevant to thermalization issues than the precise functional decay of observables. Take phase separating systems as an example. The expectation values of one-time quantities — such as the energy density (i) or observables of the type (ii) — reach equilibrium values, suggesting the equilibration of the sample at the bath temperature. This is, however, incorrect as proven by the fact that observables of type (iii), such as delayed density correlations and linear responses, decay in more than one dynamic scale, and in the slowest they do algebraically, as opposed to the typical exponential equilibrium relaxation. In spite of this, one can still define a *bona fide* effective temperature from FDRs that link correlations to their associated linear response [9] as long as one distinguishes different pairs of observables and the time-scales in which they evolve. Indeed, some observables basically ignore others — they do not interact — equilibrate quickly with the environment and are characterized by its temperature. This is the case of particle velocities. Positions, instead, do not equilibrate with the bath but acquire the same effective temperature, *i.e.*, they partially equilibrate, in their own common regime of relaxation. This notion applies to many other systems with slow dynamics and constitutes the basis of, *e.g.*, a consistent thermodynamic picture of non-equilibrium glassy dynamics as realized in mean-field theory [10]. A quantum finite-dimensional example with effective temperatures are electronic tight-binding dissipative one-dimensional models driven by external fields [11].

We explore up to which extent these ideas carry over to the non-equilibrium dynamics of a highly excited closed quantum system. For concreteness, we focus on critical quenches in which the system's parameters for times $t > 0$ are tuned to be at an equilibrium (quantum) critical point. The detailed analysis of the effective temperature based on FDRs in classical thermal quenches [10, 12] demonstrated that such a parameter has a thermodynamic meaning for very late epochs only [13], when one of the involved times is much longer than the other (see, however, Ref. [14]).

The model. To illustrate our approach, we focus on the simplest quantum integrable interacting model, the transverse field Ising chain [1]

$$\mathcal{H}_\Gamma = -J \sum_{i=1}^L (\sigma_i^x \sigma_{i+1}^x + \Gamma \sigma_i^z) \quad (1)$$

with periodic boundary conditions and even L . The Pauli matrices $\sigma_i^{x,z}$ satisfy the SU(2) algebra on the same site i and commute on different sites. In what follows we set $J, \hbar, k_B = 1$ and we measure time in units of \hbar/J and the temperature T in units of J/k_B . The model is exactly solved by a Jordan-Wigner transformation to free fermions followed by a Bogoliubov rotation in momentum space [15]. The energy of the elementary fermionic excitations with momentum k is $\epsilon_k(\Gamma) = 2[\Gamma^2 - 2\Gamma \cos k + 1]^{1/2}$. For $T = 0$ and $L \rightarrow \infty$ a quantum critical point at $\Gamma = 1$ separates a paramagnetic phase (PM, $\Gamma > 1$) with $\langle \sigma_i^x \rangle = 0$, from a ferromagnetic phase (FM, $\Gamma < 1$) with spontaneous symmetry breaking $\langle \sigma_i^x \rangle \neq 0$ and long-range order along the x direction. $\langle \sigma_i^z \rangle \neq 0$ for all $\Gamma > 0$.

The system is prepared at $t = 0$ in the ground state $|\psi_0\rangle$ of \mathcal{H}_{Γ_0} , while it subsequently evolves with $\mathcal{H}_{\Gamma=1}$, *i.e.*, at the critical point. The quench from Γ_0 to Γ injects an extensive amount of energy into the system which is henceforth conserved. After a transient (studied in Refs. [16, 17] for the chain with free boundaries) the system reaches an asymptotic stationary regime. A crucial quantity in the description of the dynamics is the difference Δ_k between the Bogoliubov angles diagonalizing \mathcal{H}_Γ and \mathcal{H}_{Γ_0} :

$$\cos \Delta_k(\Gamma, \Gamma_0) = \frac{4 [\Gamma \Gamma_0 - (\Gamma + \Gamma_0) \cos k + 1]}{\epsilon_k(\Gamma) \epsilon_k(\Gamma_0)} . \quad (2)$$

Δ_k encodes the dependence on the initial state and fixes the non-thermal statistics of the excitations created at $t = 0$.

A criterion that has been used to define an effective temperature $T_{\text{eff}}^E(\Gamma, \Gamma_0)$ is to require that the energy after the quench — quantity (i) in the Introduction — equals the average over a thermal equilibrium ensemble [1, 7]. For model (1) this implies [7]

$$0 = \int_0^\pi \frac{dk}{\pi} \epsilon_k(\Gamma) \left[\cos \Delta_k(\Gamma, \Gamma_0) - \tanh \frac{\epsilon_k(\Gamma)}{2T_{\text{eff}}^E(\Gamma, \Gamma_0)} \right] \quad (3)$$

which results in the T_{eff}^E shown in Figs. 1 and 3 with a dashed black line. Requiring, instead, the integrand in Eq. (3) to vanish defines the mode-dependent $T_{\text{eff}}^{\epsilon_k}(\Gamma, \Gamma_0)$ of the GGE [5, 6].

FDT. We focus on the symmetrized and anti-symmetrized two-time correlations of two operators A and B in the Heisenberg representation, $A_H(t) = e^{i\mathcal{H}_\Gamma t} A e^{-i\mathcal{H}_\Gamma t}$,

$$C_{\pm}^{AB}(t + t_0, t_0) = \langle \psi_0 | [A_H(t + t_0), B_H(t_0)]_{\pm} | \psi_0 \rangle, \quad (4)$$

where $[X, Y]_{\pm} \equiv (XY \pm YX)/2$. More precisely, we consider connected correlations that we still denote by C_{\pm}^{AB} . While C_+^{AB} approaches the classical correlation function for $\hbar \rightarrow 0$, C_-^{AB} is related to the linear response function R^{AB} through the Kubo formula $R^{AB}(t_1, t_0) = \delta \langle A_{H-h(t)B}(t_1) \rangle_H / \delta h(t_0) \Big|_{h=0} = (2i/\hbar) C_-^{AB}(t_1, t_0) \theta(t_1 - t_0)$ [8] which is valid in and out of equilibrium [$\theta(t < 0) = 0$ and $\theta(t > 0) = 1$]. The asymptotic stationary regime is formally defined by the limit $t_0 \rightarrow \infty$. When it is physically established depends on the observable and Γ_0 . Natural choices for A and B are the order parameter σ_i^x and the transverse magnetization σ_i^z . The σ_i^x autocorrelation functions, $C_{\pm}^x(t)$, are non-local with respect to the quasi-particles while those of σ_i^z , $C_{\pm}^z(t)$, are local in the same variables [1].

In Gibbs equilibrium at inverse temperature β the FDT connects C_+^{AB} and R^{AB} , via the model-independent time-domain and frequency-domain relations [8]

$$R^{AB}(t) = \frac{i}{\hbar} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} e^{-i\omega t} \tanh(\beta \hbar \omega / 2) \tilde{C}_+^{AB}(\omega), \quad (5)$$

$$\hbar \text{Im} \tilde{R}^{AB}(\omega) = \tanh(\beta \hbar \omega / 2) \tilde{C}_+^{AB}(\omega), \quad (6)$$

respectively. We reinstated \hbar to make the classical limit, $R^{AB}(t) = -\beta dC^{AB}(t)/dt \theta(t)$, transparent. The FDR definition of an effective temperature amounts to replacing β by $\beta_{\text{eff}}(\omega)$ in Eqs. (5) and (6) [with a t_0 -dependence in non-stationary (glassy) cases], *i.e.*,

$$\hbar \text{Im} \tilde{R}^{AB}(\omega) = \tanh[\beta_{\text{eff}}^{AB}(\omega) \hbar \omega / 2] \tilde{C}_+^{AB}(\omega) . \quad (7)$$

This is the definition that we shall repeatedly use below.

Before presenting our results let us summarize what is known about $C_{\pm}^{z,x}$ for $\Gamma = 1$. In equilibrium ($\Gamma_0 = \Gamma$) $\langle \psi_0 | \sigma_i^z(t + t_0) \sigma_i^z(t_0) | \psi_0 \rangle$ decays algebraically as $|t|^{-3/2}$ at $T = 0$ and as $|t|^{-1}$ at finite T [7]. Out of equilibrium the decay of C_+^z is $|t|^{-2}$ [16]. For the special case of a fully polarized initial condition ($\Gamma_0 = \infty$) C_-^z follows the same $|t|^{-2}$ decay, as can be inferred from the results in Ref. [2]. Instead, a generic exponential relaxation of $\langle \psi_0 | \sigma_i^x(t_0) \sigma_j^x(t_0) | \psi_0 \rangle$ was argued in [18] using semi-classical methods and later shown to hold exactly [6]. This is in contrast to the power-law decay of the $T = 0$ equilibrium order-parameter spatio-temporal correlations. As far as we know, C_-^x has not been analyzed so far. Here we complete this picture by calculating

C_{\pm}^x and C_{\pm}^z for generic Γ_0 . We also study C_{\pm}^M , where $A, B = M = \sum_{i=1}^L \sigma_i^z / L$.

The transverse local magnetization. For $\Gamma_0 \neq \Gamma = 1$ we found that C_{\pm}^z and R^z decay as a sum of power laws of t and $t+2t_0$. Thus, no characteristic time can be identified and, in addition, one cannot compare these functions to the thermal ones in order to define an effective temperature, as done in Refs. [6, 7, 17] for other observables [type (iii) of the Introduction]. Taking $t_0 \rightarrow \infty$ one finds the stationary relaxation

$$C_{\pm}^z(t) = -(8\pi t^2)^{-1} \cos 8t + \mathcal{O}(t^{-3}), \quad (8)$$

$$R^z(t) = (4\pi t^2)^{-1} [\Upsilon^{-1} - \sin 8t] + \mathcal{O}(t^{-3}), \quad (9)$$

with $\Upsilon = [(1 + \Gamma_0)/(1 - \Gamma_0)]^2$. The complementary analysis in the frequency domain allows us to define a frequency-dependent T_{eff}^z via the FDR in Eq. (7). The function $T_{\text{eff}}^z(\omega)$ is shown in Fig. 1 for $\Gamma_0 = 0.3$ as a (red) solid line and it has to be compared with the constant value obtained from Eq. (3), as in Ref. [7], shown as a black dashed line. The asymptotic regime corresponds to the limit $\omega \rightarrow 0$, zoomed in the inset, in which $\beta_{\text{eff}}^z = 1/T_{\text{eff}}^z$ diverges logarithmically with the law $-1/2(1-1/\Upsilon)/[1+(\Upsilon-2)\arctan(\sqrt{\Upsilon-1})/\sqrt{\Upsilon-1}] \ln \omega$ (green dashed line). We conclude that, although $\langle \sigma_i^z \rangle$ takes a thermal value [7], the dynamics of σ_i^z is not compatible with an equilibrium thermal behavior. For other values of Γ_0 , T_{eff}^z still vanishes at $\omega = 0$ and $\omega = \omega_{\text{max}} \equiv 8$ but it is not concave for $\Gamma_0 \gtrsim 0.35$ [19]. For increasingly narrower quenches with $\Gamma_0 \rightarrow 1$, $\beta_{\text{eff}}^z \rightarrow \infty$ uniformly over all frequencies.

The transverse global magnetization. The long-time stationary decay of the global magnetization correlations are even slower than the one of $C_{\pm}^z(t)$ [20]:

$$C_{\pm}^M(t) = (8\sqrt{\pi}t^{3/2})^{-1} \sin(8t - \pi/4) + \mathcal{O}(t^{-5/2}), \quad (10)$$

$$R^M(t) = -(4\sqrt{\pi}t^{3/2})^{-1} \cos(8t - \pi/4) + \mathcal{O}(t^{-5/2}). \quad (11)$$

The leading-order decay $t^{-3/2}$ is the same as in equilibrium at finite T . However, while the prefactor depends upon T in equilibrium [21], out of equilibrium the dependence on Γ_0 appears only at the next-to-leading order, *i.e.*, the long- t limit of $C_{\pm}^M(t)$ does not retain memory of the initial condition.

The (blue) dash-dotted line in Fig. 1 is $T_{\text{eff}}^M(\omega)$ as obtained from the FDR (7), applied to C_{\pm}^M . $T_{\text{eff}}^M(\omega)$ approaches $2/\sqrt{\Upsilon}$ at low frequencies, it vanishes for $\omega = \omega_{\text{max}}$ and becomes non-monotonic for $\Gamma_0 \gtrsim 0.27$, developing a shallow local maximum. Naively, one may expect to recover this value by treating the time-domain FDR in the long- t limit as follows. Replacing β by a constant effective value β_{eff}^* in the rhs of Eq. (5), the integral can be written as series of odd time derivatives of $C_{\pm}^M(t)$. Inserting Eqs. (10) and (11) in the rhs and lhs of this expression, respectively, yields $1 = \tanh(4\beta_{\text{eff}}^*)$ for $t \rightarrow \infty$ and therefore $T_{\text{eff}}^* = 0$. The fact that

$T_{\text{eff}}^M(\omega \rightarrow 0) \neq T_{\text{eff}}^*$ indicates that $\beta_{\text{eff}}^M(\omega)$ cannot be approximated by an average constant in the integral. Indeed, since only the derivatives of the oscillating factor in (10) contribute to the leading order of Eq. (5), T_{eff}^* is the one of the oscillatory frequency, which coincides with the threshold value ω_{max} and, for $\omega \rightarrow \omega_{\text{max}}$, β_{eff}^M diverges as $\beta_{\text{eff}}^M(\omega) \simeq -\ln(\omega_{\text{max}} - \omega)/4$. Such threshold results from the maximum of the dispersion relation and the quadratic dependence of M on the fermionic excitations. It is therefore unclear whether $T_{\text{eff}}^M(\omega = 0)$ can be recovered from the FDR in the time domain.

Interestingly enough, it turns out [19] that each frequency ω selects a mode k such that $2\epsilon_k = \omega$ and $T_{\text{eff}}^M(\omega)$ defined here from the FDR (7) coincides with the temperature $T_{\text{eff}}^{\epsilon_k}$ of the GGE.

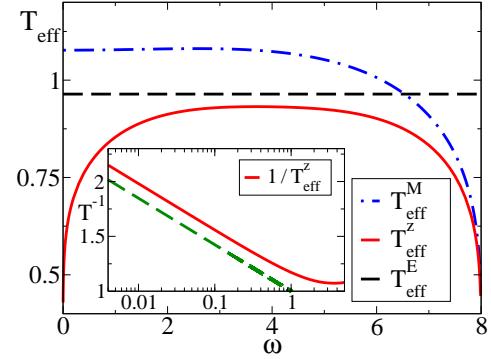


FIG. 1: (Color online.) Comparison between the effective temperature defined via the frequency-domain FDR applied to σ_i^z (red solid line) and M (blue dash-dotted line), and the energy definition (black dashed horizontal line) for $\Gamma_0 = 0.3$. The inset highlights the logarithmic divergence of $T_{\text{eff}}^z(\omega)$ for $\omega \rightarrow 0$.

The order parameter. Equations (8), (9), (10) and (11) are invariant under $\Gamma_0 \mapsto \Gamma_0^{-1}$ because $\cos \Delta_k(1, \Gamma_0) = \cos \Delta_k(1, \Gamma_0^{-1})$ [see Eq. (2)] is the sole quantity bringing about the dependence on Γ_0 in the stationary limit $t_0 \rightarrow \infty$ of $C_{\pm}^{M,z}$ [19]. In the same limit and for $\Gamma = 1$ we find numerically that this invariance also holds for C_{\pm}^x . Henceforth we restrict to quenches originating from the FM phase. We computed C_{\pm}^x for a chain with $L = 10^3$ and $t_0 = 10$ with the methods employed in Refs. [7, 15, 16]. Our numerical results are fitted very accurately by

$$C_{\pm}^x(t) \simeq e^{-\frac{t}{\tau}} A_C [1 + a_C t^{-\frac{1}{2}} \sin(4t + \phi)], \quad (12)$$

$$R^x(t) \simeq e^{-\frac{t}{\tau}} A_R [1 - a_R t^{-\frac{1}{2}} \cos(4t + \phi)], \quad (13)$$

with (numerically) the same rate τ^{-1} as the one $\tau^{-1} = -\int_0^\pi (dk/\pi) [d\epsilon_k(\Gamma)/dk] \ln \cos \Delta_k$ analytically proved [6] to characterize the exponential long-time decay of $\langle \psi_0 | \sigma_i^x(t) \sigma_j^x(t) | \psi_0 \rangle$. The expression for τ finds further support from the fact that with the substitution $\cos \Delta_k \rightarrow \tanh(\beta \epsilon_k/2)$ one recovers the equilibrium τ_{eq} [22, 23] in this as well as other statistical averages. Although several fitting parameters are involved in

Eqs. (12) and (13), we tested these expressions in various instances and they turned out to be always remarkably accurate already for $t \gtrsim 5$ [19]. In Fig. 2 we show C_+^x and R^x for $\Gamma_0 = 0.3$, together with a zoom into the long-time decay and its comparison with the leading exponential decay in the upper inset. The lower inset confirms the high quality of the fit of the correction terms to the forms given in Eqs. (12) and (13) which are actually indistinguishable from the data. The non-equilibrium coherence time $\tau = \pi\sqrt{\Upsilon-1}/[4\arctan(\sqrt{\Upsilon-1})]$ decreases upon increasing $|1-\Gamma_0|$, *i.e.*, the energy injected into the system and $\tau \sim |1-\Gamma_0|^{-1}$ for $\Gamma_0 \rightarrow 1$. While the parameters $A_{R,C}$ depend on Γ_0 , their ratio $A_C/A_R = 1.210(5)$ does not within our numerical accuracy. More details on the fitting parameters of the oscillating (lattice) correction will be presented in Ref. [19].

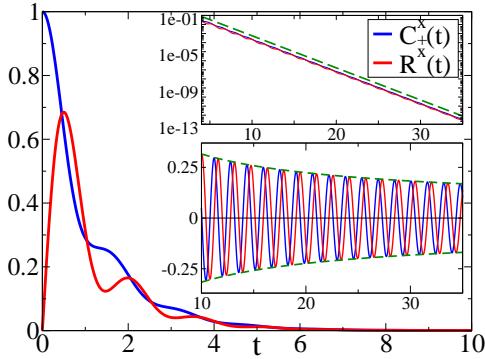


FIG. 2: (Color online.) Decay of the order-parameter correlation C_+^x (blue line) and the linear response R^x (red line) for $\Gamma_0 = 0.3$. Upper inset: zoom into the long- t decay that demonstrates the exponential relaxation with the characteristic time τ defined in the text (dashed green line). Lower inset: $(e^{t/\tau} C_+^x / A_C - 1) / a_C$ and $(e^{t/\tau} R^x / A_R - 1) / a_R$ vs. t ; the green dashed line is the $t^{-1/2}$ envelope of the damped oscillations, in agreement with Eqs. (12) and (13).

The effective temperatures determined in the frequency and in the time domain are equivalent in this case. As discussed above, replacing β by a constant β_{eff}^x , turns the rhs of the FDT (5) in the time domain into a series of time derivatives of $C_+^x(t)$ which yields

$$\hbar A_R / (2A_C) = \tan(\hbar\beta_{\text{eff}}^x / 2\tau) \quad (14)$$

for $t \rightarrow \infty$, *i.e.*, neglecting the oscillatory corrections in Eqs. (12) and (13). Alternatively, Eq. (7) yields $\beta_{\text{eff}}^x(\omega = 0) = \int_0^\infty dt t R(t) / \int_0^\infty dt C(t)$ for $\omega \rightarrow 0$ which numerically coincides with the constant value in Eq. (14). For $\hbar\beta_{\text{eff}}^x / 2\tau \ll 1$ one recovers the classical limit $\beta_{\text{eff}}^x \simeq -R^x(t)/[dC^x(t)/dt] \simeq \tau A_R / A_C$. All three determinations of T_{eff}^x are shown in Fig. 3 as functions of Γ_0 and they are compared to T_{eff}^E (dashed line) from Eq. (3) [7].

We completed our analysis by studying space-dependent correlations and we found that they yield anal-

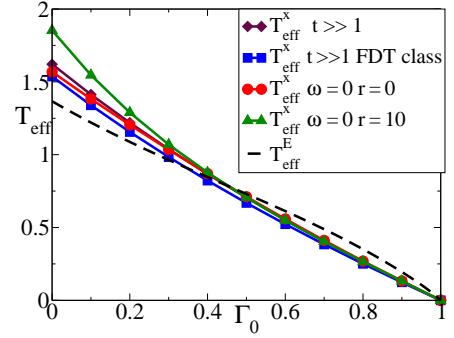


FIG. 3: (Color online.) Γ_0 dependence of the order-parameter effective temperature T_{eff}^x compared to T_{eff}^E defined from the energy [see Eq. (3)] (dashed line). The solid lines, from bottom to top, indicate the values determined on the basis of the classical limit of the FDR in the time domain, of the limit $\omega \rightarrow 0$ of the frequency-domain FDR, of Eq. (14), and of the limit $\omega \rightarrow 0$ of the frequency-domain FDR but for spins separated by a distance $r = 10$. The dependence on Γ_0 can be read from the one of τ and Eq. (14).

ogous results, as shown in Fig. 3 for the x -component of two spins at distance $r = 10$. (Note that differently from case $r = 0$ shown in Fig. 2, correlations with $r \neq 0$ display a light-cone effect due to the finite speed of the quasi-particles [6, 17–19].)

Conclusions. Independently of the functional form of the correlations involved, the FDRs allow us to define various effective temperatures. We calculated the (self) FDR for three observables that are local ($\sigma_i^{x,z}$) or non-local (M) in space and local (σ_i^z, M) or non-local (σ_i^x) in the quasi-particles. σ_i^z is not compatible with Gibbs thermal equilibrium at any effective temperature. The frequency-domain FDR for M yields a finite $T_{\text{eff}}^M(\Gamma_0)$ in the limit $\omega \rightarrow 0$. Frequency and time-domain determinations of $T_{\text{eff}}^x(\Gamma_0)$ are equivalent. T_{eff}^M and T_{eff}^x have the same qualitative dependence on Γ_0 but they differ (also from T_{eff}^E). This excludes a single temperature effective Gibbs description (as the one discussed in Ref. [24]) of the full stationary dynamics of this model but the question remains as to whether some of the temperatures which emerge can be attributed a thermodynamic meaning.

We finally stress that a *bona fide* thermal behavior should be accompanied by the validity of suitable FDTs also in the context of quantum quenches.

Acknowledgments. We thank F. Igloi, G. Santoro, G. Semerjian, A. Silva, F. Zamponi for discussions. A. Gambassi and L. F. Cugliandolo thank LPTHE and ICTP, respectively, for hospitality during the preparation of this work that was financially supported by ANR-BLAN-0346 (FAMOUS) and CNRS.

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